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16. ABSTRACT

This paper reports the results of a project to develop a methodology for incorporating uncertainty analysis as an integral part of the water quality modeling process. The model used for demonstrating this methodology is the EPA-supported water quality model QUAL2E. The QUAL2E model was chosen for this application because it is a general purpose computer code that is widely used by state regulatory agencies in waste load allocation and other environmental planning activities. The resulting uncertainty model is named QUAL2E-UNCAS.

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UNCERTAINTY ANALYSIS USING QUAL2E

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OBJECTIVE

Uncertainty analysis has been the subject of much discussion in the ecosystem modeling literature (Rose and Swartzman, 1981 and O'Neill and Gardner, 1979). In the water resources literature, lake eutrophication models have been used to compare various methods of uncertainty analysis (Reckhow, 1979; Scavia et al., 1981; and Malone et al., 1983). A systematic approach to uncertainty analysis for general purpose stream water quality models has yet to appear, and thus is not available to most model users.

This paper reports the results of a project to develop a methodology for incorporating uncertainty analysis as an integral part of the water quality modeling process. The model used for demonstrating this methodology is the EPA supported water quality model QUAL2E (Brown and Barnwell, 1985). The QUAL2E model was chosen for this application because it is a general purpose computer code, widely used by consultants and state regulatory agencies in waste load allocation and other planning activities. The resulting uncertainty model is named QUAL2E-UNCAS.

The more frequently reported uncertainty analysis strategies include sensitivity analysis, first order error analysis, and monte carlo simulation. In normal usage, sensitivity analysis is accomplished using a one variable-at-a-time approach (Duke, 1976). Sensitizing more than one input variable at a time is an attractive method for assessing their interaction effects on the output variable. However, when many input parameters and variables are altered, the number of combinations to be investigated becomes large, thus complicating interpretation of the results. Experimental design strategies can be efficiently applied in this situation.

First order error analysis utilizes the first order approximation to

the relationship for computing variances in multivariate situations. The input variables are assumed to act independently (covariances are ignored) and the model to be linear (the higher order terms of the Taylor expansion are omitted). The first order approximation to the components of output variance is often good (Walker, 1982). Monte carlo simulation is a method for numerically operating a complex system which has random components. Input variables are sampled at random from pre-determined probability distributions (with or without correlation) and the distribution of output values from repeated simulations is analyzed statistically. The validity of this method is not affected by nonlinearities in the water quality model.

QUAL2E-UNCAS

The methodology reported in this work allows the model user to perform uncertainty analysis with relative ease and efficiently manages the output from the analysis. Although the application is specific to the QUAL2E model, the methodology is general. The preprocessing and postprocessing algorithms used are, in principle, applicable to many water quality models. The preprocessor allows the user to select the variables and/or parameters to be altered, without having to manually restructure the input data set. This task is performed automatically by the preprocessor for as many uncertainty conditions as the user wishes to simulate. The postprocessor stores and manipulates only the output of interest, thus reducing potential voluminous output. The user must select the important variables and/or locations in the stream network where uncertainty effects are desired. The output analysis may be for variables at a specific location or for the maximum/minimum of important variables, regardless of their location.

Three uncertainty analysis techniques can be employed in QUAL2E-UNCAS; sensitivity analysis, first order error analysis, or monte carlo simulation. The input specification options and output characteristics accompanying each technique are summarized below.

Input Specifications	Output Characteristics
1. Sensitivity Analysis	
a) One variable at a time	Sensitivity Matrix
*single, multiple levels	
b) Multiple variables, levels	Experimental Design,
*factorial design	Main/Interaction Effects
2. First Order Error Analysis	
*levels of input variable(s)	Sensitivity Matrix
*input variances	Components of Variance Matrix
3. Monte Carlo Simulation	
*probability distributions	Summary Statistics,
*mean, variance, covariance	Frequency Distributions

The user is provided this array of options for flexibility, because the methods differ in their assumptions and will not always agree with each other. Discrepancies may be explained by errors in the first order approximation, or by errors due to biased variance calculations. Monte carlo simulation has the advantage of output frequency distributions, but it carries a high computational burden. First order error propagation provides a direct estimate of model sensitivity, but that variability is usually more indicative of the variance of model components rather than of the dynamics of the model structure.

EXAMPLE APPLICATION - OUACHITA RIVER BASIN

The data used to demonstrate the capabilities of QUAL2E-UNCAS were obtained from an NCASI study of the Ouachita River Basin in 1980 (NCASI, 1982). In this study, water quality simulations were examined for portions of a deep, low velocity river where algal dynamics and benthal phenomena were important. A schematic representation of the system is shown in Figure 1, and a plot of observed and predicted dissolved oxygen concentrations is presented in Figure 2. Point loads are predominantly located in the upper half of the basin and the river receives both municipal and industrial wastewater flows.

FIRST ORDER ERROR ANALYSIS (FOEA)

The QUAL2E-UNCAS output for first order error analysis consists of two parts, (a) a tabulation of sensitivity coefficients and (b) a listing of the components of variance. The sensitivity coefficients represent the percent change in the output variable resulting from a one per cent (1%) change in each input variable. The components of variance for each output variable Y, are the percentage of output variance attributable to each input variable X, computed in the following manner.

$$\mathrm{Var}(Y_j) = \sum_i \mathrm{Var}(X_i)(\Delta Y_j/\Delta X_i)^2$$

Each term in the summation is a component of the variance of the output variable, Y_j contributed by the input variable, X_i. The components of the output variance, $\mathrm{Var}(Y_j)$, represent a weighting of the input variances, $\mathrm{Var}(X_i)$, by the square of the sensitivity of model output to input $(\Delta Y_j/\Delta X_i)$.

Tables 1 through 4 show the FOEA results for the output variables of CBOD and DO, at three locations in the Ouachita system; an upstream location (RM 220), a midpoint location (RM 172), and a downstream location (RM 120).

For the CBOD sensitivity coefficients shown in Table 1, it is clear that the input forcing functions dominate the model sensitivity. Point load and headwater flows and CBOD have by far the largest sensitivity coefficients in the upstream portion of the basin (RM 220). At the

downstream location (RM 120) the situation changes. The point load forcing function sensitivities remain strong, and are joined by high sensitivity to temperature and the CBOD oxidation rate coefficient. The headwater forcing function sensitivities are of diminished importance in the lower reaches of the basin.

Table 2 presents the components of variance for the modeled CBOD output. These results show a similar, though somewhat modified pattern to the sensitivity data in Table 1. The headwater and pointload flows and CBOD are the dominant contributors to CBOD variability in the upper reaches of the basin (RM 220). The variance contributions from the CBOD rate coefficient, temperature, and velocity grow in importance as one proceeds through the system. In the downstream portion of the basin, the variance contributions from the headwater forcing functions are small, as one would expect.

The sensitivity coefficients and components of variance results midway in the basin (RM 172) clearly show the upstream to downstream transition of dominant inputs. The total variability in output CBOD estimated by FOEA, when expressed as a standard deviation, increases in the direction of flow from 0.27 mg/L to 0.43 mg/L.

The FOEA results for dissolved oxygen are shown in Tables 3 and 4. As contrasted with CBOD, only the headwater forcing function inputs (Table 3), rather than both the headwater and point load forcing functions, contribute in a major way to DO variability. At RM 220 practically all the sensitivity in modeled DO can be attributed to the headwater DO, however as one proceeds downstream, the modeled dissolved oxygen looses its sensitivity to headwater DO. In the lower reaches of the basin, flow, velocity, depth and temperature have the highest sensitivity coefficients, followed by the biochemical factors of CBOD oxidation, SOD, ammonia oxidation, and the algal respiration and oxygen production factors. These results indicate that for this system, the hydraulic and temperature inputs play a more substantial role than the biochemical parameters in affecting the uncertainty in modeled dissolved oxygen values. Note that the effect of atmospheric reaeration on DO variability is manifest in the velocity and depth input variables.

Similar patterns of dissolved oxygen sensitivity are shown in Table 4 which contains the components of variance analysis. The role of headwater dissolved oxygen is striking, as is the increasing importance of SOD as the major contributor to dissolved oxygen variability in the lower reaches of the basin. The profound influence of SOD results from both its large sensitivity coefficient and its large input uncertainty. The hydraulic inputs and temperature have a major effect on DO variability at RM 120, while the effects of ammonia and CBOD oxidation, and algal dynamics remain at a modest level compared to SOD.

The total variability in dissolved oxygen computed in FOEA increases in the downstream direction, varying from 0.38 mg/L to 0.53 mg/L when expressed as a standard deviation.

MONTE CARLO SIMULATION

The monte carlo simulation computations provide summary statistics for state variables at specific locations in the basin. Tables 5 and 6 contain the mean, minimum, maximum, range, standard deviation, coefficient of variation, and skew coefficient for simulated CBOD and DO at the upstream, mid-point, and downstream locations in the Ouachita Basin.

Comparison of the monte carlo generated standard deviations with those computed in the FOEA shows fairly good agreement. The similarity of these values indicates that CBOD and DO in this system are not particularly non-linear over the range of uncertainties assumed in the simulations

The frequency distributions generated by the monte carlo analysis are shown graphically in Figures 3 and 4 for CBOD and DO respectively. (Note the distributions are plotted to a scale given by the magnitude of the standard deviation). The distributions become more dispersed as one proceeds downstream and the DO distribution appears to exhibit some kurtosis in the lower reaches of the basin.

SUMMARY

The following observations summarize experience to date with uncertainty analysis using QUAL2E.

1. QUAL2E-UNCAS provides a useful framework for performing uncertainty analysis in steady state water quality modeling.

2. Application of this methodology to a data set from the Ouachita River Basin has highlighted some of the interesting features of uncertainty analysis.

    a. Importance of hydraulics, forcing functions, and benthal phenomena.

    b. Changing sensitivities and components of variance in different portions of the river basin.

    c. Utility of probability distributions of the state variables.

3. Input variance and probability density functions are needed for more confident application of this technique. Compiling an input variance data base has a high priority.

4. QUAL2E-UNCAS has potential as a useful tool in water quality management and resource allocation.

5. Refinements to the QUAL2E-UNCAS model are continuing.

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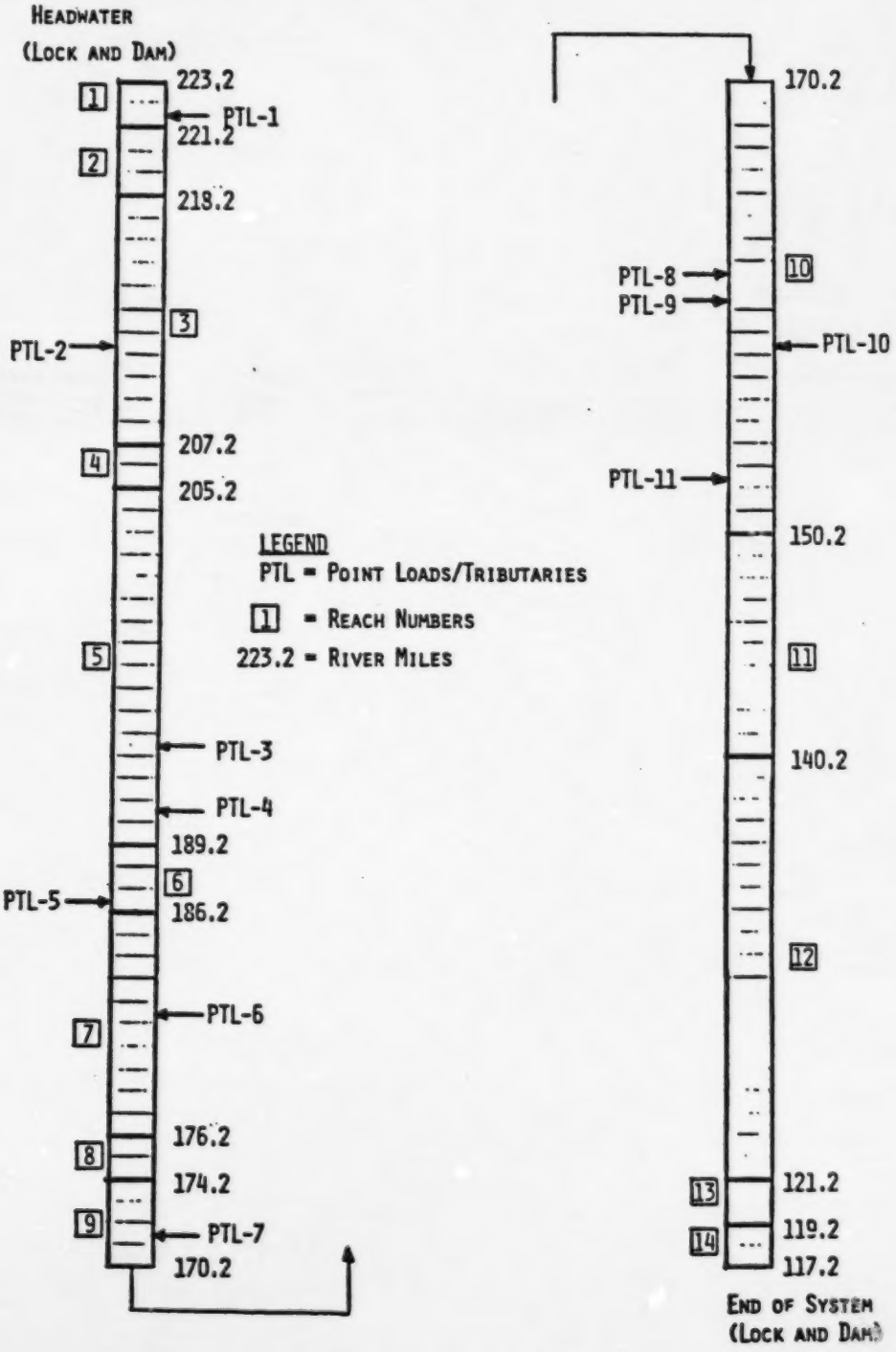

Figure 1. OUACHITA RIVER BASIN SCHEMATIC

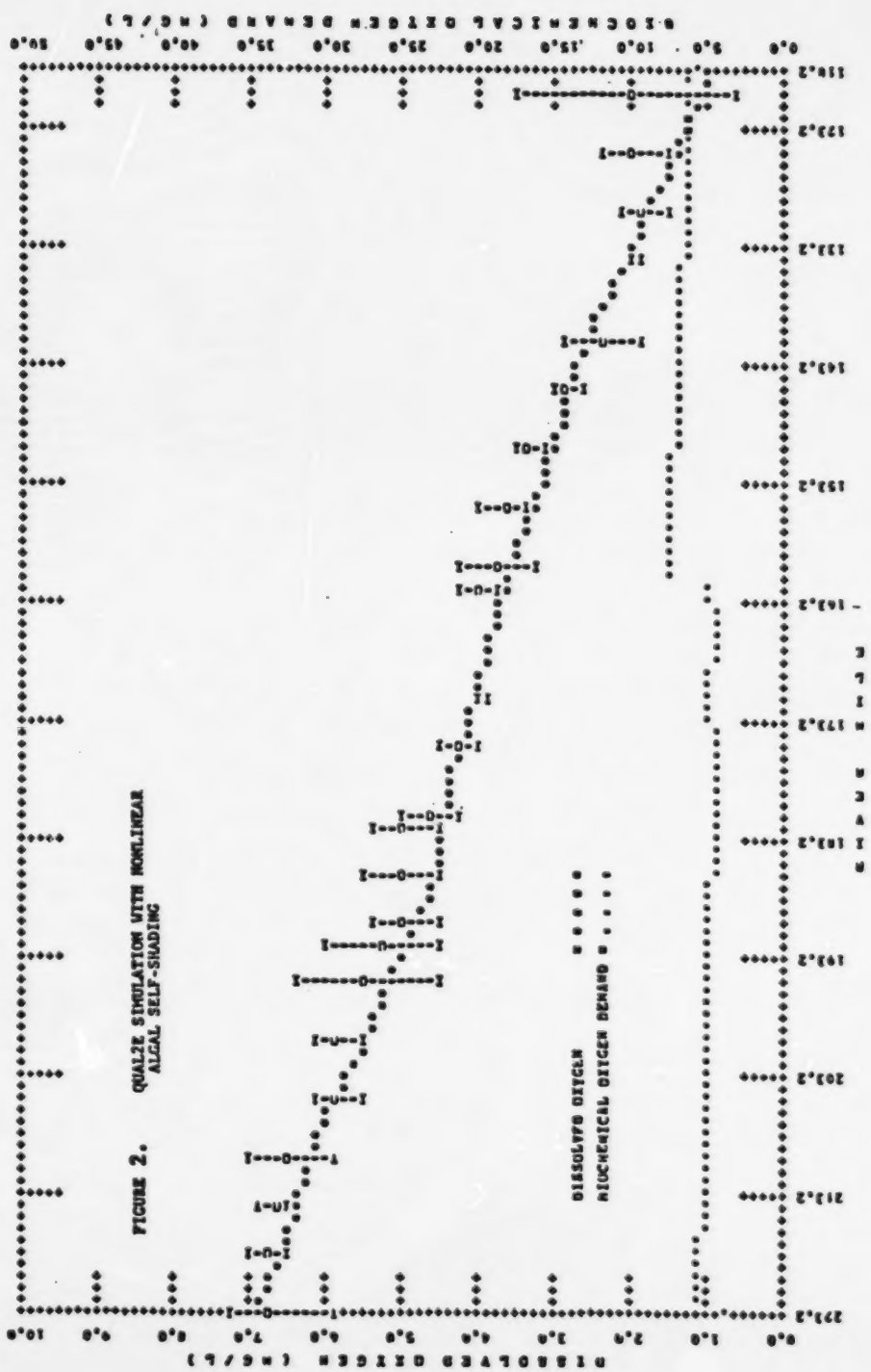
QUALZE SIMULATION WITH NONLINEAR ALGAL SELF-SHADING
DISSOLVED OXYGEN
BIOCHEMICAL OXYGEN DEMAND
DISSOLVED OXYGEN (MG/L)
BIOCHEMICAL OXYGEN DEMAND (MG/L)
METERS

FIGURE 2.

TABLE 1

Q U A L 2 E - U N C A S

FIRST ORDER ERROR ANALYSIS
OUTPUT VARIABLE : BOD

OUACHITA RIVER EXAMPLE - JULY 1980 SURVEY

INPUT VARIABLE	SENSITIVITY COEFFICIENTS RM 220	RM 172	RM 120
Temp Coef, k_1	-.01 (8)*	-.11 (8)	-.22 (7)
Velocity	.02 (7)	.18 (6)	.36 (5)
k_1	-.02 (6)	-.19 (5)	-.37 (4)
Temperature	-.05 (5)	-.46 (3)	-.90 (1)
HW Flow	-.28 (4)	-.12 (7)	-.17 (8)
HW BOD	.67 (1)	.48 (2)	.29 (6)
PTL Flow	.31 (3)	.31 (4)	.54 (3)
PTL BOD	.33 (2)	.52 (1)	.71 (2)

* ( ) = rank, 1 = highest

TABLE 2

Q U A L 2 E - U N C A S

FIRST ORDER ERROR ANALYSIS

OUTPUT VARIABLE : BOD

OUACHITA RIVER EXAMPLE - JULY 1980 SURVEY

INPUT VARIABLE (Std. Dev.)	COMPONENTS OF VARIANCE (%) RM 220	RM 172	RM 120
Velocity (5%)	0.0	3.3	6.8
k_1 (10%)	0.2	14.2	28.8
Temp. (2%)	0.0	3.4	6.8
HW Flow (4%)	5.4	1.0	1.0
HW BOD (6%)	70.2	32.4	6.3
PTL Flow (4%)	6.7	6.2	10.0
PTL BOD (6%)	17.3	39.0	34.0
TOTALS			
Variance	.075	.065	.186
Std. Dev. (mg/L)	.27	.26	.43

TABLE 3

Q U A L 2 E - U N C A S

FIRST ORDER ERROR ANALYSIS

OUTPUT VARIABLE : DO

OUACHITA RIVER EXAMPLE - JULY 1980 SURVEY

INPUT VARIABLE	SENSITIVITY COEFFICIENTS RM 220	RM 172	RM 120
NH3OXYUP	-.01 (7)*	-.18 (8)	-1.67 (5)
AGYOXYPR	.01 (8)	.19 (7)	1.24 (8)
AGYOXYUP	-.01 (9)	-.14 (9)	-1.09 (10)
Velocity	.04 (4)	.39 (4)	3.20 (3)
Depth	-.00 (11)	-.28 (5)	-1.83 (4)
k_1	-.02 (6)	-.14 (10)	-1.22 (9)
SOD	-.02 (5)	-.27 (6)	-1.44 (6)
Benthal Ammonia Rate	.00 (10)	-.09 (11)	1.35 (7)
Temperature	-.15 (2)	-1.12 (1)	-7.66 (1)
HW Flow	.05 (3)	.47 (2)	3.69 (2)
HW DO	.92 (1)	.43 (3)	.86 (20)

* ( ) = rank, 1 = highest

TABLE 4

QUAL2E - UNCAS

FIRST ORDER ERROR ANALYSIS

OUTPUT VARIABLE : DO

OUACHITA RIVER EXAMPLE - JULY 1980 SURVEYS

INPUT VARIABLE (STD. DEV.)	COMPONENTS OF VARIANCE (%) RM 220	RM 172	RM 220
3 Algae/Ammonia (5%) Oxygen Parameters	0	3	6
Velocity (5%)	0	6	11
Depth (5%)	0	3	4
k_1 (10%)	0	3	7
SOD Rate (20%)	0	44	36
Benthal Ammonia (10%)	0	1	8
Temperature (2%)	0	8	10
HW Flow (4%)	0	5	10
HW DO (6%)	99	14	1
TOTALS			
Variance	.142	.109	.283
Std. Dev. (mg/L)	.38	.35	.53

TABLE 5

Q U A L 2 E - U N C A S

MONTE CARLO SUMMARY

OUACHITA RIVER EXAMPLE - JULY 1980 SURVEY

	BOD (mg/L)		
STATISTIC	RM 220	RM 172	RM 120
Base Mean	5.73	5.09	6.29
Sim. Mean	5.73	5.09	6.32
Minimum	5.09	4.39	5.26
Maximum	6.27	5.70	7.34
Range	1.18	1.31	2.08
Std. Dev.	0.23	0.24	0.43
Coef. Var (%)	4.0	4.7	6.8
Skew Coef.	-0.18	-0.12	-0.06
Comparison:			
Std. Dev. from			
FOEA	0.27	0.26	0.43

TABLE 6

Q U A L 2 E - U N C A S

MONTE CARLO SUMMARY

OUACHITA RIVER EXAMPLE - JULY 1980 SURVEY

	DISSOLVED OXYGEN (mg/L)		
STATISTIC	RM 220	RM 172	RM 120
Base Mean	6.77	4.13	1.12
Sim. Mean	6.83	4.23	1.24
Minimum	5.86	3.10	0.00
Maximum	7.50	5.14	2.71
Range	1.64	2.04	2.71
Std. Dev.	0.34	0.32	0.49
Coef. Var %	4.9	7.6	39.4
Skew Coef.	-0.27	-0.20	0.06
Comparison:			
Std. Dev. from FOEA	0.38	0.33	0.53

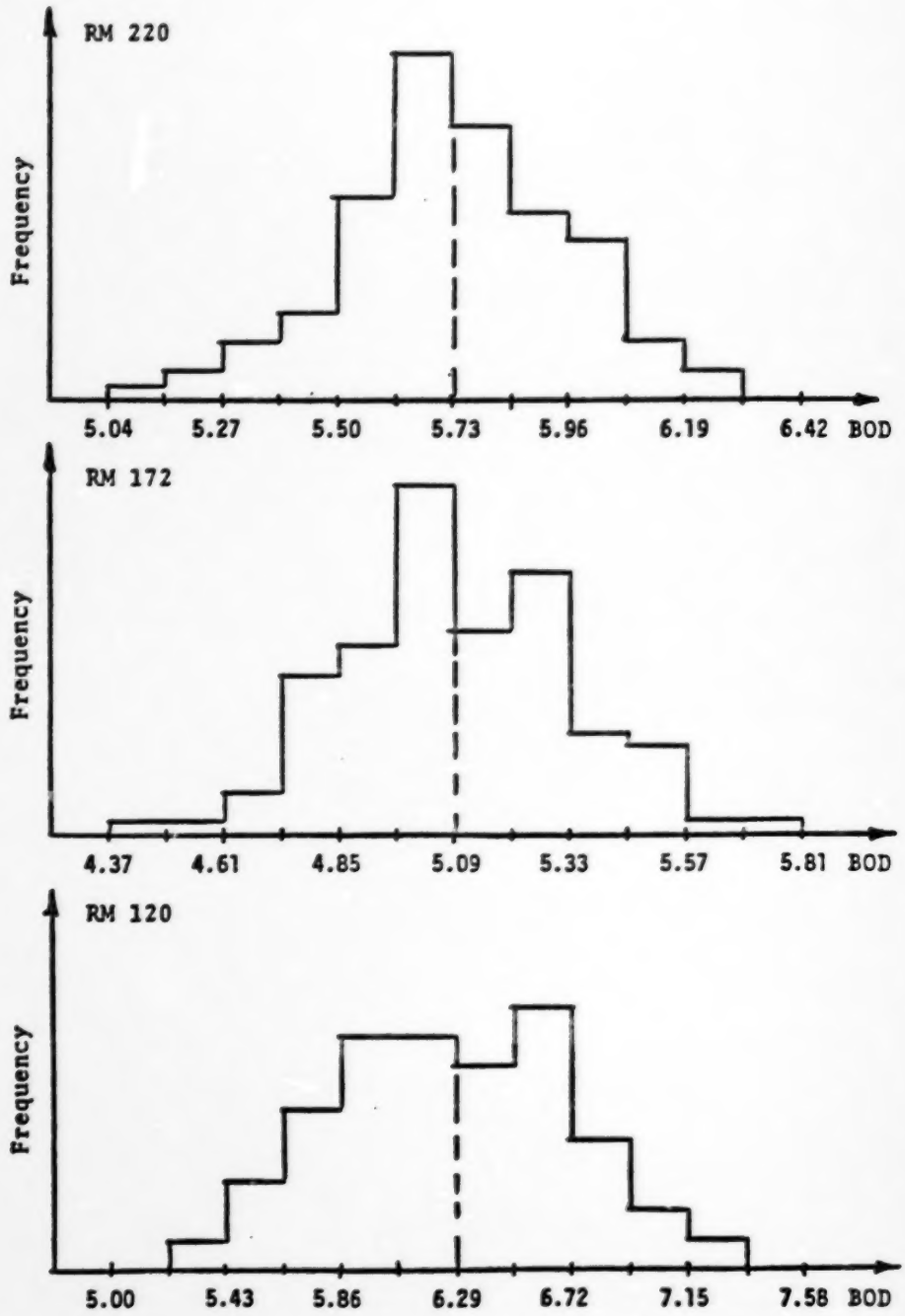

Figure 3. MONTE CARLO SIMULATIONS - BOD

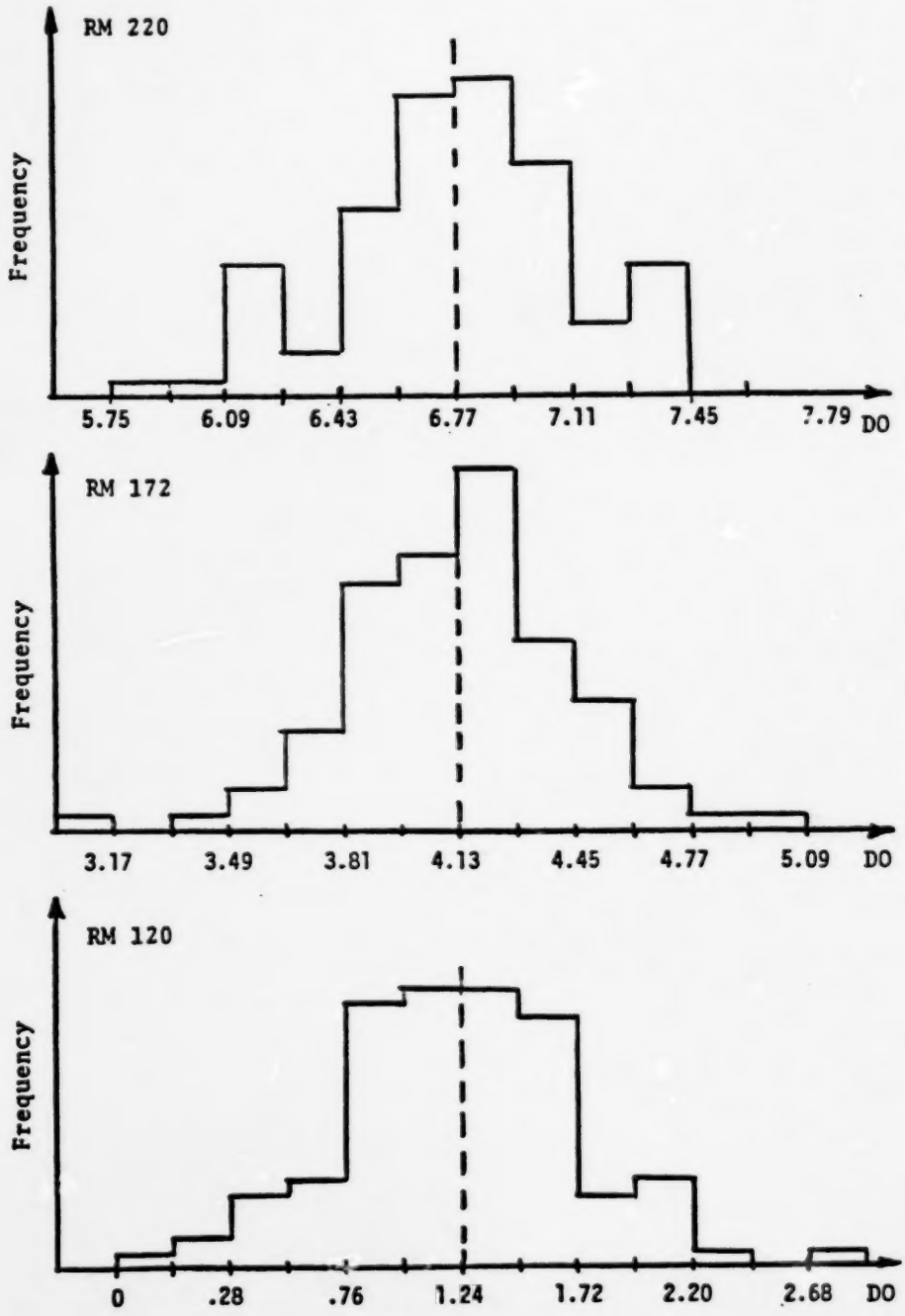

Figure 4. MONTE CARLO SIMULATIONS - DISSOLVED OXYGEN